PHYSICAL REVIEW E **69**, 065401(R) (2004)

Collective modes of quasi-two-dimensional Yukawa liquids

Z. Donkó,[1] P. Hartmann,[1] and G. J. Kalman[2]
[1]Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary
[2]Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA

(Received 30 October 2003; published 1 June 2004)

Particles in dusty plasmas are often confined to a quasi-two-dimensional arrangement. In such layers—besides the formation of compressional and (in-plane) shear waves—an additional collective excitation may also show up, as small-amplitude oscillations of the particles perpendicular to the plane are also possible. We explore through molecular dynamics simulations the properties (fluctuation spectra, dispersion relation, Einstein frequency) of this out-of-plane transverse mode in the strongly coupled liquid phase of Yukawa systems.

DOI: 10.1103/PhysRevE.69.065401 PACS number(s): 52.27.Gr, 52.27.Lw, 82.70.−y

Layered structures of charged particles are well known to occur in particle traps [1] and complex — e.g., dusty—plasmas [2]. Depending on the conditions of the experiments these systems often exhibit structural changes. The structural phase transitions in one-dimensional (1D) and 2D systems, relevant to particle traps, have theoretically been studied by Dubin [3], while Totsuji *et al.*[4] investigated the formation of layers in Yukawa systems confined by a one-dimensional force field.

The properties of waves in the *crystalline* phase of 2D (single layer) Yukawa systems have thoroughly been investigated both theoretically and experimentally [5]. The collective excitations in 2D Yukawa *liquids* have recently been studied by Murillo and Gericke [6] and by Kalman *et al.* [7]. The ideal 2D systems exhibit two collective modes: the compressional (longitudinal, $\mathcal{L}$) mode and the shear (transverse, $\mathcal{T}$) mode. While the previous studies addressed only the case of an ideal two-dimensional layer, the present study is devoted to *quasi-two-dimensional* systems where the particles form a layer of finite width. Such a situation is found, e.g., in dusty plasmas, where the particles in the layer are levitated due to the balance between the gravitational force and the electrostatic force originating from the sheath electric field. (On the other hand, our system is still idealized due to the neglect of effects such as ion wakes [8,9] that appear in dusty plasmas.) In the one-dimensional potential well formed by the confinement the particles can also move perpendicularly to the plane. The aim of the present Rapid Communication is to explore the properties of the additional (out-of-plane transverse, $\mathcal{P}$) collective mode associated with this type of motion, in the *strongly coupled liquid phase* of the system. Studies of this mode in *plasma crystals* have recently been reported by Qiao and Hyde [10]. It is noted that in the case of 1D Yukawa chains [11] the corresponding mode has been referred to as an "optical" mode [12].

An ideal two-dimensional system can fully be characterized by (i) the plasma coupling parameter $\Gamma=(Q^2/4\pi\varepsilon_0)\times(1/ak_BT)$ and (ii) the screening parameter $\kappa=a/\lambda_D$, where Q is the charge of the particles, T is the temperature, $a=1/\sqrt{n\pi}$ is the Wigner-Seitz (WS) radius, n is the areal density of particles, and λ_D is the Debye (screening) length of the Yukawa potential:

$$\phi(r)=\frac{Q^2}{4\pi\varepsilon_0}\frac{\exp(-r/\lambda_D)}{r}. \quad (1)$$

It is noted that in experimental papers a often denotes the distance of nearest neighbors, in contrast with the present definition.

In our quasi-2D system the particles can freely move in the (x,y) plane while a confinement potential $V_c(z)\propto z^2$ acts upon them when they are displaced from the $z=0$ plane; see Fig. 1. The confinement force is given in the form

$$F_z=-f_0cz, \quad (2)$$

where the amplitude f_0 is the third characteristic parameter of the system. The constant c is set in a way that at $f_0=1$ the confinement force at a "vertical" displacement $z=a$ equals the absolute value of the force between two Coulomb particles separated by a—i.e., $F_z(z=a)=-Q^2/4\pi\varepsilon_0a^2$.

We follow the motion of particles by molecular dynamics simulation based on the particle-particle particle-mesh (PPPM) algorithm [13], modified for the Yukawa potential. The simulation domain is a three-dimensional cubic box with periodic boundary conditions. The box is, however, only partially filled with particles due to the external confinement, which keeps them near the $z=0$ plane (as shown in Fig. 1). In the PPPM method the interparticle force is partitioned into (i) a force component F_{PM} that can be calculated on a mesh (the "mesh force") and (ii) a short-range force F_{PP}, which is to be applied to closely separated pairs of particles only (for more details see [13]). This way the PPPM method makes it

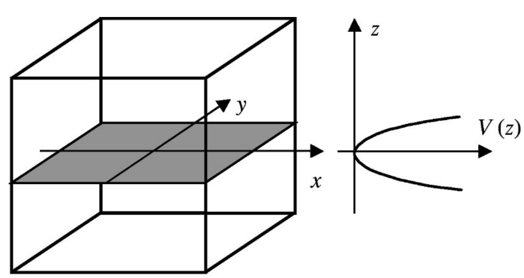

FIG. 1. The 1D parabolic $V(z)$ potential confines the particles in the vicinity of the shaded region (quasi-2D plane) of the cubic simulation box.

possible to take into account periodic images of the system (in the PM part), without truncating the long-range Coulomb or low-κ Yukawa potentials. (For high κ values the PP part alone provides sufficient accuracy; in these cases the mesh part of the calculation is not used.) The equations of motion of the particles are integrated using the leapfrog scheme, with a typical time step of $\omega_{p3}\Delta t \approx 1/40$, where ω_{p3} is the three-dimensional plasma frequency (note that the particles move in 3D space). The number of simulation particles is chosen to be $N=1600$. This systems size proved to be sufficiently large, as verified by checking calculations using $N=6400$ particles. The desired system temperature is reached by rescaling the particle momenta during the initialization phase of the simulation. The system temperature does not show an observable drift during the subsequent measurement phase of the simulation, following the initialization period. The measurements on the system are taken at constant volume (V), particle number (N), and total energy (E). The results are presented for $\Gamma=100$ and for a wide range of κ values. The system is in a strongly coupled liquid phase for the whole domain of the parameter values studied here.

Information about the (thermally excited) collective modes and their dispersion is obtained from analysis of the correlation spectra of the longitudinal and (in-plane as well as out-of-plane) transverse current fluctuations [$\lambda(k,t)$, $\tau(k,t)$, and $\pi(k,t)$, respectively]:

$$\lambda(k,t) = k\sum_j v_{jx}(t)\exp[ikx_j(t)],$$

$$\tau(k,t) = k\sum_j v_{jy}(t)\exp[ikx_j(t)],$$

$$\pi(k,t) = k\sum_j v_{jz}(t)\exp[ikx_j(t)], \tag{3}$$

where x_j and v_j are the position and velocity of the jth particle. Here we assume that k is directed along the x axis [the system is isotropic in the (x,y) plane] and accordingly omit the vector notation of the wave number. The data are stored and subsequently Fourier analyzed [14] for a series of wave numbers, which are multiples of $k_{\min}=2\pi/H$, where H is the edge length of the simulation box.

The number of layers formed in the system depends on the strength of the confinement. Figure 2(a) shows the distribution of particle density along the z direction, $F(z)$, for different strengths of confinement (f_0), $\Gamma=100$, and $\kappa=0.27$. We observe the transition from a two-layered configuration to a single layer at $f_0 \approx 1.4$. Due to the finite temperature of the system, the layers do not resemble crystal planes (like in ion trap experiments) but they are rather broad. At $f_0 \approx 1.4$ the width of the layer is $\approx 0.86a$ (at half of the maximum of the distribution). Doubling the amplitude of the potential results in a width $0.17a$. When the repulsion between the particles decreases at higher κ values, the potential with the same amplitude results in a stronger confinement. Thus, with increasing κ the number of layers, or the width of the single layer, decreases (in agreement with the observation of Totsuji *et al.* [4]), as illustrated in Fig. 2(b). Our further studies of the dynamical properties concern the domain of parameters when a *single layer* is formed. At a higher number of layers the mode structure is expected to be more complicated [15,16] but this is not within the scope of the present paper.

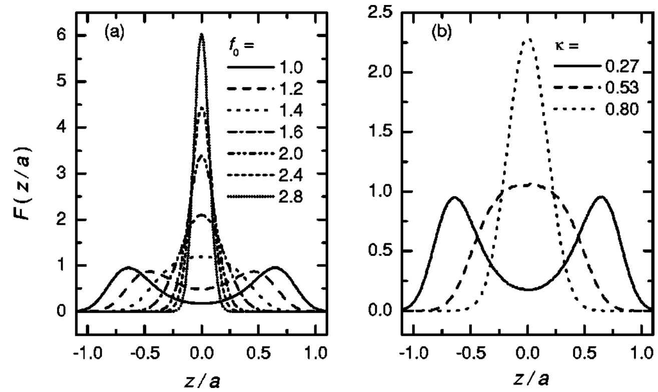

FIG. 2. Density distribution of particles along the z direction [normalized as $\int F(z/a)d(z/a)=1$]. (a) Dependence on the strength of confinement at $\Gamma=100$ and $\kappa=0.27$ and (b) dependence on κ at constant $f_0=1.0$.

Representative current fluctuation spectra for all the three ($\mathcal{L}$, $\mathcal{P}$, and $\mathcal{T}$) modes are illustrated in Fig. 3, for $\Gamma=100$, $\kappa=0.27$ and $\kappa=1.33$, and $f_0=2.0$. The frequency is normalized by the nominal 2D plasma frequency $\omega_0=(Q^2n/2\varepsilon_0 ma)^{1/2}$, where m is the mass of particles. (Note that ω_0 may also have different definitions in other works.)

Considering the $\mathcal{L}$ mode, we can observe sharp peaks in the $L(k,\omega)$ spectra, as in the case of (ideal) 2D Coulomb and Yukawa systems [6,7,17]. Peaks in the $\mathcal{T}$ mode spectra [see Figs. 3(e) and 3(f)] show up only above a certain (cutoff) wave number, similarly to the case of 3D Yukawa systems [18]. The $\mathcal{P}$ mode posseses a finite frequency at $k=0$. At small wave numbers the peaks of the spectra shift to lower ω as $\bar{k}$ is increased ($\bar{k}=ka$). The width of the peaks of the $P(k,\omega)$ spectra narrows as f_0 is increased, which is an indication of an increasing lifetime of this collective excitation.

The dispersion relations derived from the spectra are displayed in Fig. 4 for different values of f_0 and κ. The plasma coupling parameter is $\Gamma=100$ for all the graphs. At constant κ, as shown in Fig. 4(a), the frequency of the out-of-plane transverse mode changes significantly as the strength of the confinement force f_0 is varied. The $\mathcal{L}$ and $\mathcal{T}$ modes are relatively unaffected by the value of f_0. The frequency of these modes is somewhat smaller at $f_0=1.4$, which is near the lower bound of f_0 for the formation of a single layer [see Fig. 2(a)]. It is noted that at lower f_0 values, when two layers are formed, two longitudinal and two in-plane transverse modes appear, similarly to those identified in the classical (ideal) bilayer system [15]. Additionally, two out-of-plane transverse modes are also formed in the two-layered system, which are also believed to be in-phase and out-of-phase modes (when particles in the two layers oscillate in phase or with a phase difference of 180° in the two layers). The $\mathcal{L}$ mode exhibits a quasiacoustic behavior, with a linear portion of the dispersion curve around $k=0$, which widens with increasing κ, as can be seen in Fig. 4(b). The $\mathcal{T}$ mode shows an

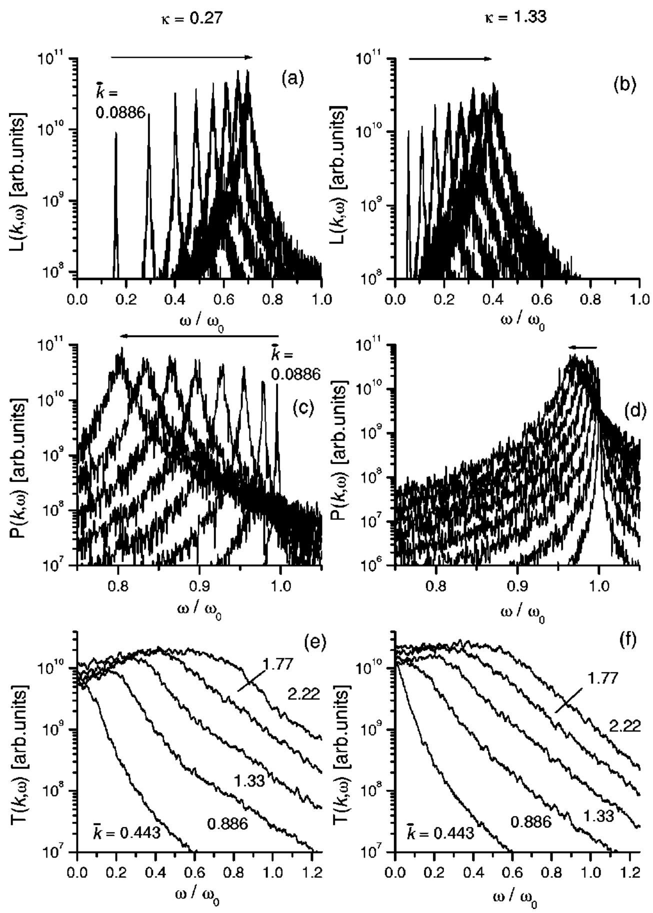

FIG. 3. Spectra of current fluctuation of the $\mathcal{L}$ mode (a),(b), $\mathcal{P}$ mode (c),(d), and the $\mathcal{T}$ mode (e),(f). $\kappa=0.27$ for (a),(c),(e) and $\kappa=1.33$ for (b),(d),(f). (a),(b),(c),(d) show the spectra for eight different wave numbers, multiples of the smallest wave number $\overline{k}=2\pi a/H=0.0886$; the arrows show increasing $\overline{k}$ values. (e),(f) show the $T(k,\omega)$ spectra for higher wave numbers, indicated in the plots.

acoustic, $\omega \sim k$ dispersion, with a cutoff at a finite wave number.

For the $\mathcal{P}$ mode $\mathrm{d}\omega/\mathrm{d}k<0$ in the $\overline{k}\lesssim 2.1$ domain. The frequency of the mode slightly increases towards higher wave numbers. At $k=0$ the whole layer oscillates in unison in the potential well with a frequency $\omega(k=0)=\sqrt{f_0 c/m}$, which gives

$$\frac{\omega(k=0)}{\omega_0}=\sqrt{f_0/2}. \tag{4}$$

A decreasing confinement force amplitude results in a smaller $\omega(k=0)$ and $\omega(k\to\infty)$. At a constant f_0 the value of $\omega(k=0)$ does not change when κ is varied, but—as shown in Fig. 4(b)—$\omega(k>0)$ increases with increasing κ. This is explained by the decreased interparticle force (at an average particle separation) at higher κ. The dispersion properties of the $\mathcal{P}$ mode are rather similar to the corresponding collective mode of a linear chain of particles [11].

The frequency of the out-of-plane transverse mode at high wave numbers ($k\to\infty$ limit—in other words, the Einstein frequency [19]) can be calculated by considering the forces acting upon a single particle displaced in the z direction, while all other particles are in rest in the $z=0$ plane. The force is the sum of the confining force and the force due to repulsion of the other particles, $F(z)=-f_0cz+F_\mathrm{r}(z)$. The $F_\mathrm{r}(z)$ repulsive force can be calculated as $F_\mathrm{r}(z)=-\partial V_\mathrm{r}/\partial z$, where $V_\mathrm{r}(z)$ is the potential distribution due to a charge distribution $\rho(x,y)$ in the $z=0$ plane. In our calculations $\rho(x,y)$ is obtained either from the radial (2D) pair correlation function (PCF) or by taking the particles at hexagonal lattice sites in the $z=0$ plane. The $F_\mathrm{r}(z)$ force was found to be a nearly linear function of the displacement z, in the $|z|<0.3a$ domain, where the particle displacement is expected to fall. The resulting (Einstein) frequency (when the particles in the $z=0$ plane are situated at lattice sites) is

$$\frac{\omega_\mathrm{E}}{\omega_0}=\frac{\omega(k\to\infty)}{\omega_0}\cong\sqrt{\frac{f_0-1.63\,\exp(-1.37\kappa)}{2}}. \tag{5}$$

In the case of using the disordered configuration in the $z=0$ plane instead of lattice sites (through PCF's obtained in the

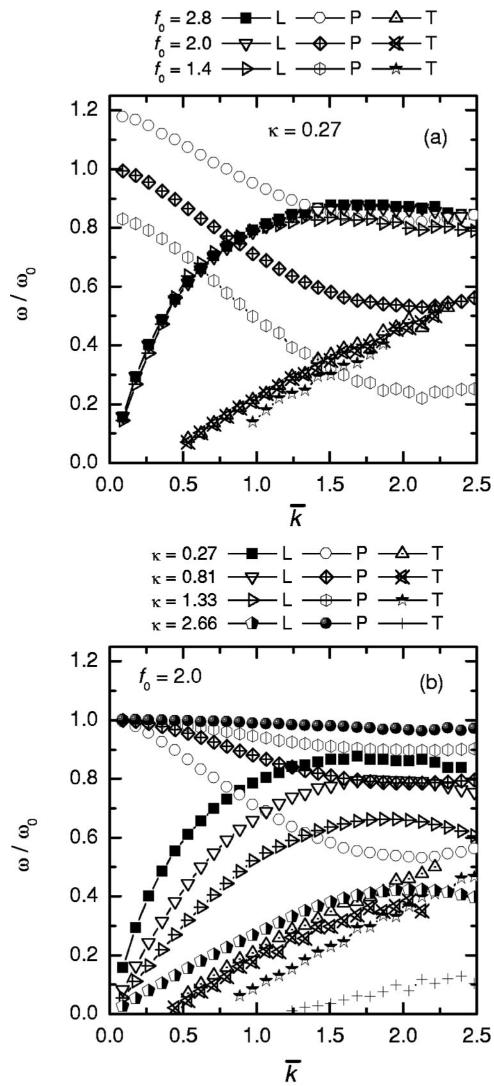

FIG. 4. Dispersion of the $\mathcal{L}$, $\mathcal{P}$ and $\mathcal{T}$ modes at $\Gamma=100$. (a) $\kappa=0.27$ and different values of the confining force amplitude f_0 and (b) $f_0=2.0$ and different values of the screening parameter κ.

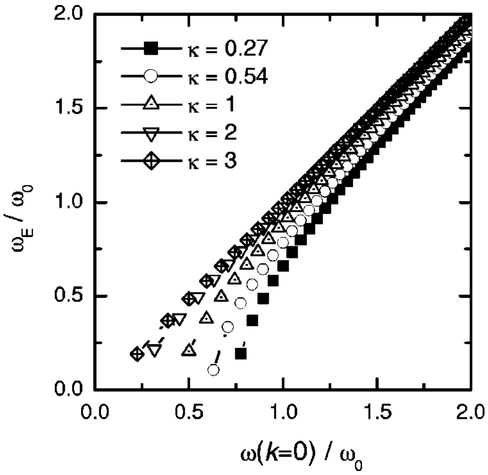

FIG. 5. Einstein frequency of out-of-plane oscillations as a function of $\omega(k=0)/\omega_0$, for different values of κ.

liquid state simulations), a frequency very close to that given by Eq. (5) is obtained. Figure 5 shows the Einstein frequency (5) as a function of $\omega(k=0)/\omega_0$. At low values of κ the value of ω_E is significantly lower than $\omega(k=0)$. In the high-κ limit the two frequencies are equal, as the screening becomes very strong and the particles interact very weakly. In this case the frequency of the $\mathcal{P}$ mode becomes nearly independent of $\bar{k}$, as can actually be seen in Fig. 4(b).

The lifetime of the collective excitations is inversely proportional to the widths of the peaks of the current fluctuation spectra (shown in Fig. 3). Our results indicate that only the excitations with the smallest wave numbers can propagate a distance comparable to, or longer than, the size of the computational box (H). These modes could, in principle, feel the finite size of the computational box. However, calculations carried out with 4 times higher particle number ($N=6400$) give the same dispersion relations within the limit of errors, as those using $N=1600$ particles.

In conclusion, we have studied the spectra and dispersion characteristics of collective excitations of strongly coupled Yukawa liquids confined by an external (1D) parabolic potential, in the domain of the system parameters where a single layer with finite width is formed. In addition to the well-known longitudinal (compressional) and (in-plane) transverse modes, which exhibit the same behavior as observed in ideal 2D systems, we explored the properties of the out-of-plane transverse ($\mathcal{P}$) mode. The $\mathcal{P}$ mode was found to have (i) a finite frequency $\omega(0)$ at $k=0$, being defined by the amplitude of the confining potential; (ii) a negative $d\omega/dk$ at small $\bar{k}$, which, however, changes to slightly positive above $\bar{k}\approx 2.1$; (iii) a weaker dependence of ω on k with increasing κ (in the limit of high screening values ω becoming independent of k); and (iv) an Einstein frequency (ω_E), which, at small screening, is significantly smaller than $\omega(0)$, but in the limit of high screening $\omega_E=\omega(0)$.

Support through Grant Nos. OTKA-T-34156, MTA-NSF-OTKA-028, NSF-PHYS-0206695, NSF-INT-0002200, and DE-FG02–03ER54716 is gratefully acknowledged. Z.D. thanks G. Bánó for his comments on the manuscript.

[1] T. B. Mitchell, J. J. Bollinger, D. H. E. Dubin, X.-P. Huang, W. M. Itano, and R. H. Bundham, Science **282**, 1290 (1998); J. J. Bollinger, T. B. Mitchell, X.-P. Huang, W. M. Itano, J. N. Tan, B. M. Jelenković, and D. J. Wineland, Phys. Plasmas **7**, 7 (2000).
[2] A. Melzer, V. A. Schweigert, I. V. Schweigert, A. Homann, S. Peters, and A. Piel, Phys. Rev. E **54**, R46 (1996); J. B. Pieper, J. Goree, and R. A. Quinn, J. Vac. Sci. Technol. A **14**, 519 (1996); M. Zuzic *et al.*, Phys. Rev. Lett. **85**, 4064 (2000); A. Homann, A. Melzer, S. Peters, R. Madani, and A. Piel, Phys. Lett. A **242**, 173 (1998).
[3] D. H. E. Dubin, Phys. Rev. Lett. **71**, 2753 (1993).
[4] H. Totsuji, T. Kishimoto, Y. Inoue, C. Totsuji, and S. Nara, Phys. Lett. A **221**, 215 (1996).
[5] S. Nunomura, D. Samsonov, and J. Goree, Phys. Rev. Lett. **84**, 5141 (2000); S. Nunomura, J. Goree, S. Hu, X. Wang, A. Bhattacharjee, and K. Avinash, *ibid.* **89**, 035001 (2002); S. Nunomura, J. Goree, S. Hu, X. Wang, and A. Bhattacharjee, Phys. Rev. E **65**, 066402 (2002); K. Avinash, P. Zhu, V. Nosenko, and J. Goree, *ibid.* **68**, 046402 (2003).
[6] M. S. Murillo and D. O. Gericke, J. Phys. A **36**, 6273 (2003).
[7] G. J. Kalman, P. Hartmann, Z. Donkó, and M. Rosenberg, Phys. Rev. Lett. **92**, 065001 (2004).
[8] M. Lampe, G. Joyce, G. Ganguli, and V. Gavrishchaka, Phys. Plasmas **7**, 3851 (2000).
[9] A. V. Ivlev, U. Konopka, G. Morfill, and G. Joyce, Phys. Rev. E **68**, 026405 (2003).
[10] K. Qiao and T. W. Hyde, Phys. Rev. E **68**, 046403 (2003).
[11] S. Nunomura, T. Misawa, N. Ohno, and S. Takamura, Phys. Rev. Lett. **83**, 1970 (1999); T. Misawa, N. Ohno, K. Asano, M. Sawai, S. Takamura, and P. K. Kaw, *ibid.* **86**, 1219 (2001).
[12] Bin Liu, K. Avinash, and J. Goree, Phys. Rev. Lett. **91**, 255003 (2003).
[13] R. W. Hockhey and J. W. Eastwood, *Computer Simulation Using Particles* (McGraw-Hill, New York, 1981).
[14] J.-P. Hansen, I. R. McDonald, and E. L. Pollock Phys. Rev. A **11**, 1025 (1975); S. Hamaguchi, Plasmas Ions **2**, 57 (1999).
[15] Z. Donkó, G. J. Kalman, P. Hartmann, K. I. Golden, and K. Kutasi, Phys. Rev. Lett. **90**, 226804 (2003); Z. Donkó, P. Hartmann, G. J. Kalman, and K. I. Golden, J. Phys. A **36**, 5877 (2003).
[16] G. J. Kalman, Z. Donkó, and K. I. Golden, Contrib. Plasma Phys. **41**, 191 (2001); K. I. Golden and G. J. Kalman, J. Phys. A **36**, 5865 (2003).
[17] H. Totsuji and H. Kakeya, Phys. Rev. A **22**, 1220 (1980).
[18] H. Ohta and S. Hamaguchi, Phys. Rev. Lett. **84**, 6026 (2000); M. S. Murillo, *ibid.* **85**, 2514 (2000).
[19] Z. Donkó, P. Hartmann, and G. J. Kalman, Phys. Plasmas **10**, 1563 (2003); B. Bakshi, Z. Donkó, and G. J. Kalman, Contrib. Plasma Phys. **43**, 261 (2003).